LCF Seminar Series

What is a 200,000 CPUs Petaflop Computer Good For (a Theoretical Chemist Perspective)?

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10:00 a.m., Building 4500N, Weinberg Auditorium

Abstract:
We describe the efforts undertaken to efficiently parallelize the computational chemistry code NWChem on the Cray XT hardware using the Global Arrays/ARMCI middleware. We show how we can now use 200K+ processors to address complex scientific problems.

Bio:
Edoardo Aprà has been a research scientist at the Oak Ridge National Laboratory (ORNL) with the Computational Chemical Sciences Group in the Computer Science and Mathematics Division since 2006. Edoardo Aprà's research activity focuses on activities related to high performance computational algorithm and software development as well as the use of this software in chemical applications. Edoardo earned his Ph.D. in Physical Chemistry at the University of Turin in 1993 while collaborating at the software development of the quantum chemistry computer code CRYSTAL. After a two year post-doctoral appointment at Pacific Northwest National Laboratory (PNNL), he joined the faculty of the Material Sciences Department of the University of Milan in 1996. Edoardo returned to PNNL in 1998, assuming the position assuming the position of task lead for the development of the massively parallel software NWChem in 2003.

Host: Ricky Kendall, kendallra@ornl.gov (865-576-6905)